Predictions of the Solubility of Acid Gases in Monoethanolamine (MEA) and Methyldiethanolamine (MDEA) Solutions Using the Electrolyte-UNIQUAC Model

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Abstract

A thermodynamic model was developed for representing vapor-liquid equilibria of the CO_2-H_2S-MEA-MDEA-water system. The model accounts for chemical equilibria in the liquid phase and physical equilibria between the liquid and vapor phases. Activity coefficients are represented by the Electrolyte-UNIQUAC equation. The present extension uses an ion-pair interaction approach and satisfies both the principles of like-ion repulsion and local electroneutrality. Contributions from long-range ion-ion interactions are represented by a Debye-Hückel formula suitable for mixed solvents, water and alkanolamines. Adjustable parameters of the Electrolyte UNIQUAC equation, representing short-range binary interactions, were determined by data regression using binary, ternary, and quaternary system VLE data. Predicted H_2S and CO_2 vapor pressures are in good agreement with the reported experimental data for aqueous solutions of a single acid gas as well as mixtures of H_2S and CO_2 in MEA and MDEA and their mixtures in the temperature range 25 to 120°C.

Keywords: hydrogen sulfide, carbon dioxide, alkanolamines, vapor liquid equilibria, Electrolyte UNIQUAC model

Introduction

The removal of CO_2 and H_2S from gas streams is an important operation in the natural gas and synthetic ammonia industries, oil refineries, and petrochemical plants. Absorption/stripping with aqueous solutions of alkanolamines is the major industrial technology that has been developed since the 1930's (Kohl and Nielson, 1997). Design of gas treating processes with alkanolamine-based aqueous solvents requires knowledge of the vapor-liquid equilibria (VLE) of the CO_2-H_2S-alkanolamine-water system. A large body of experimental VLE data has been reported in the literature. Representation of these data with a suitable thermodynamic model is required. An accurate model is essential for process simulation and design of gas treating operations.

Early thermodynamic models adopted empirical approaches that did not account for physical interactions. Kent and Eisenberg [1] proposed a model that neglects activity coefficients and uses apparent equilibrium constants in the equations of chemical equilibria. Deshmukh and Mather [2] developed a more rigorous thermodynamic model. Except for water, all activity coefficients were calculated using the Guggenheim equation. Weiland and coworkers [3] provided values for the interaction parameters of the model for most of the commercially important amine systems. Later, a similar model was proposed by Li and Mather [4]. The Guggenheim equation was replaced by the well-known Pitzer model to calculate the activity coefficients.

Austgen et al. [5,6] treated the amine-water system as a mixed solvent of variable composition. Activity coefficients are represented with the electrolyte-NRTL model [7,8] treating both long-range electrostatic interactions and short-range binary interactions. Adjustable

parameters of the model, representing short-range binary interactions, were provided for several commercially important amine systems.

The objective of the present work is to develop a thermodynamically rigorous VLE model that represents CO_2 and/or H_2S solubility data reported in the literature for aqueous solutions of MEA, MDEA, and mixtures of MEA and MDEA, in order that it could be used with confidence to calculate the equilibrium distribution of species, molecular and ionic, in the highly nonideal liquid phase. This would make the equilibrium model useful in the context of a rate-based model for speciation of the bulk liquid phase.

An Extended UNIQUAC Model for the Excess Gibbs Energy of Electrolyte Systems

The approach taken assumes that the excess Gibbs energy of electrolyte systems can be considered as the sum of two terms, one related to long-range forces between ions and the other to short-range forces between all species. The Debye-Hückel formula is used to represent the contribution from long-range ion-ion interactions while the UNIQUAC equation is adopted to compute the contribution from short-range interactions of all kinds. The CO_2-H_2S-alkanolamine-water system is comprised of molecules and ions, which differ appreciably in both size and shape. Unlike other local composition models, the UNIQUAC model has the distinct advantage of giving consideration to molecular size and shape through structural parameters. Cristensen et al. [9] and Sander et al. [10] were the first to use a modified UNIQUAC model for electrolyte systems. In reformulating the UNIQUAC equation, they adopted Chen's like ion repulsion assumption, but chose not to adopt the concept of local electroneutrality. This formulation results in adjustable energy parameters of the model that are ion-specific, unlike the parameters of Chen's Electrolyte-NRTL model, which are ion-pair-specific. In the present work it is assumed that short range interactions occur between ion pairs with surface area fractions

randomly distributed relative to those of the individual ions, resulting in ion-pair specific interaction parameters. This greatly simplifies the resulting activity coefficient expressions, relative to the NRTL electroneutrality model, yet avoids the excessive number of parameters of the ion specific UNIQUAC model. Expressions for the electrolyte UNIQUAC activity coefficients of the various species in the liquid phase are needed. These expressions are readily available [10] and reported elsewhere [11]. The activity coefficients of the various components in the electrolyte system due to short-range and long-range contributions are calculated as follows:

(i) For a solvent component *n*,

$$\ln g_n = \ln g_n^{dh} + \ln g_n^{C} + \ln g_n^{R} \tag{1}$$

(ii) For a molecular solute *m*,

$$\ln g_m^{*} = \ln g_m^{dh} + \ln g_m^{*,C} + \ln g_m^{*,R} \tag{2}$$

(iii) For an ionic component *i*,

$$\ln g_i^{*} = \ln g_i^{*,dh} + \ln g_i^{*,C} + \ln g_i^{*,R} \tag{3}$$

A Thermodynamic Framework for Calculating Vapor Liquid Equilibria for the CO_2-H_2S-MEA-MDEA-Water System

The CO_2 and H_2S from the gas phase that dissolve into the liquid react partially with the amines to produce a number of ionic species. Ionic species are treated as nonvolatile and the vapor pressures of amines are assumed negligible in the temperature range under consideration. The following equilibrium reactions exist in solution:

(i) Ionization of water:

$$2\ H_2O \overset{K_w}{\rightleftharpoons} H_3O^{+} + OH^{-} \tag{4}$$

(ii) Dissociation of carbon dioxide:

$$CO_2 + 2\,H_2O \overset{K_{CO_2}}{\rightleftharpoons} HCO_3^- + H_3O^+ \tag{5}$$

(iii) Dissociation of bicarbonate:

$$HCO_3^- + H_2O \overset{K_{HCO_3^-}}{\rightleftharpoons} H_3O^+ + CO_3^{--} \tag{6}$$

(iv) Dissociation of hydrogen sulfide:

$$H_2S + H_2O \overset{K_{H_2S}}{\rightleftharpoons} H_3O^+ + HS^- \tag{7}$$

(v) Dissociation of bisulfide:

$$H_2O + HS^- \overset{K_{HS^-}}{\rightleftharpoons} H_3O^+ + S^{--} \tag{8}$$

(vi) Dissociation of protonated MEA:

$$RNH_3^+ + H_2O \overset{K_{b,MEA}}{\rightleftharpoons} RNH_2 + H_3O^+ \tag{9}$$

(vii) Dissociation of protonated MDEA:

$$RR'R''NH^+ + H_2O \overset{K_{b,MDEA}}{\rightleftharpoons} RR'R''N + H_3O^+ \tag{10}$$

(viii) MEA carbamate reversion to bicarbonate:

$$RNHCOO^- + H_2O \overset{K_{CRBM}}{\rightleftharpoons} RNH_2 + HCO_3^- \tag{11}$$

From these reactions, the following equilibrium relations can be written:

$$K_w = \frac{x_{H_3O^+}\, x_{OH^-}}{x_{H_2O}^2} \frac{g^*_{H_3O^+}\, g^*_{OH^-}}{g^2_{H_2O}} \tag{12}$$

$$K_{CO_2} = \frac{x_{H_3O^+}\, x_{HCO_3^-}}{x_{H_2O}^2\, x_{CO_2}} \frac{g^*_{H_3O^+}\, g^*_{HCO_3^-}}{g^2_{H_2O}\, g^*_{CO_2}} \tag{13}$$

$$K_{HCO_3^-} = \frac{x_{H_3O^+}\, x_{CO_3^{--}}}{x_{H_2O}\, x_{HCO_3^-}} \frac{g^*_{H_3O^+}\, g^*_{CO_3^{--}}}{g_{H_2O}\, g^*_{HCO_3^-}} \tag{15}$$

$$K_{H_2S} = \frac{x_{H_3O^+}\, x_{HS^-}}{x_{H_2O}\, x_{H_2S}} \frac{g^*_{H_3O^+}\, g^*_{HS^-}}{g_{H_2O}\, g^*_{H_2S}} \tag{15}$$

$$K_{\mathrm{HS^-}} = \frac{x_{\mathrm{H_3O^+}}\, x_{\mathrm{S^{--}}}}{x_{\mathrm{H_2O}}\, x_{\mathrm{HS^-}}} \frac{g^*_{\mathrm{H_3O^+}}\, g^*_{\mathrm{S^{--}}}}{g_{\mathrm{H_2O}}\, g^*_{\mathrm{HS^-}}} \tag{16}$$

$$K_{\mathrm{b,MEA}} = \frac{x_{\mathrm{H_3O^+}}\, x_{\mathrm{RNH_2}}}{x_{\mathrm{H_2O}}\, x_{\mathrm{RNH_3^+}}} \frac{g^*_{\mathrm{H_3O^+}}\, g_{\mathrm{RNH_2}}}{g_{\mathrm{H_2O}}\, g^*_{\mathrm{RNH_3^+}}} \tag{17}$$

$$K_{\mathrm{b,MDEA}} = \frac{x_{\mathrm{H_3O^+}}\, x_{\mathrm{RR'R''N}}}{x_{\mathrm{H_2O}}\, x_{\mathrm{RR'R''NH^+}}} \frac{g^*_{\mathrm{H_3O^+}}\, g_{\mathrm{RR'R''N}}}{g_{\mathrm{H_2O}}\, g^*_{\mathrm{RR'R''NH^+}}} \tag{18}$$

$$K_{\mathrm{CRBM}} = \frac{x_{\mathrm{HCO_3^-}}\, x_{\mathrm{RNH_2}}}{x_{\mathrm{H_2O}}\, x_{\mathrm{RNHCOO^-}}} \frac{g^*_{\mathrm{HCO_3^-}}\, g_{\mathrm{RNH_2}}}{g_{\mathrm{H_2O}}\, g^*_{\mathrm{RNHCOO^-}}} \tag{19}$$

Expressions for these constants as function of temperature were taken from Austgen et al. [5,6]. Activity coefficients of all species are assumed to be independent of pressure. Dielectric constants of the amine solvents are obtained from Austgen et al. [5]. Combining MEA, MDEA, CO_2, H_2S, and H_2O mass balances, with the electroneutrality condition, the mole fraction summation equation and the equations above results in a set of 15 nonlinear equations in 15 unknowns, the mole fractions of the various species in the liquid phase, ionic and molecular, and the ratio n_W / n_T.

For the molecular solutes, CO_2 and H_2S, physical equilibrium is expressed by

$$y_m \phi_m P = x_m g^*_m H^{(P^s_w)}_{m,w} \exp \frac{\bar{v}^{\infty}_{m,w}(P - P^s_w)}{RT} \tag{20}$$

where $H^{(P^s_w)}_{m,w}$ is Henry's constant at the system temperature and the saturation pressure of water, P is the system pressure, P^s_w is the vapor pressure of pure liquid water at the system temperature T, and $\bar{v}^{\infty}_{m,w}$ is the partial molal volume of the molecular solute m at infinite dilution in water.

For water, vapor-liquid equilibria may be expressed by

$$y_{H_2O}\, j_{H_2O}\, P = x_{H_2O}\, g_{H_2O}\, j^{s}_{w}\, P^{s}_{w} \exp \frac{v^{l}_{w}(P - P^{s}_{w})}{RT} \tag{21}$$

In this equation, j^{s}_{w} is the fugacity coefficient of saturated water at the system temperature and v^{l}_{w} is the molar volume of pure liquid water at the system temperature.

The correlation of Brelvi and O'Connell [12] was used to estimate the partial molar volumes of CO_2 and H_2S at infinite dilution in water. Molar volumes and vapor pressures of pure water were obtained from a polynomial fit to data from the steam tables. The vapor-phase fugacity coefficients in Eqs. 20 and 21 were calculated by using the Redlich-Kwong-Soave equation of state. All values used in the model are reported in Kaewsichan [11].

Interaction Parameters

For the CO_2-H_2S-MEA-MDEA-water system there are three solvent species, two molecular solutes, and 9 ionic species. The following are the ion pairs present in our system at significant levels: RNH_3^+ $RNHCOO^-$, RNH_3^+ HCO_3^-, RNH_3^+ HS^-, $RR'R''H^+$ HCO_3^-, $RR'R''H^+$ HS^-, and $RR'R''H^+$ $RNHCOO^-$. For other ion pairs the concentrations of H_3O^+, OH^-, CO_3^{--}, and S^{--} ions are so small that ion pairs associated with these species may be neglected. In forming ion pairs it is assumed that the anions will randomly distribute around a cation and vice versa. This results in the following surface area fraction of an ion pair:

$$q_{z_a c\, z_c a} = q_a \frac{z_c x_c}{\sum_{c'} z_{c'} x_{c'}} + q_c \frac{z_a x_a}{\sum_{a'} z_{a'} x_{a'}} \tag{22}$$

where $\sum_{c'}$ and $\sum_{a'}$ mean summation over all cations and anions, respectively.

The surface area parameter of an ion pair, $q_{z_a c\, z_c a}$, is readily calculated from the following simple relation:

$$q_{z_a c\, z_c a} = z_a q_c + z_c q_a \tag{23}$$

The residual activity coefficients of the molecular components and the ion pairs are readily calculated using this approach from Equation 21.

The residual activity coefficients of the ions are related to the residual activity coefficients of the corresponding ion pairs via the relation:

$$\ln g^{*,R}_{z_a c\, z_c a} = \frac{z_a}{z_a + z_c} \ln g^{*,R}_{c} + \frac{z_c}{z_a + z_c} \ln g^{*,R}_{a} \tag{24}$$

To accomplish a solution to Eq. (24), it is reasonable to assume for each ion pair that $g^{*,R}_{c}$ is equal to $g^{*,R}_{a}$. This gives

$$2 \ln g^{*,R}_{z_a c\, z_c a} = \ln g^{*,R}_{c} = \ln g^{*,R}_{a} \tag{25}$$

Equation (25) represents the relationship between the activity coefficient of an ion pair and those of the individual ions. Combining these results to obtain the ionic activity coefficients:

$$\left\langle \ln g^{*,R}_{c} \right\rangle = \sum_{a} \left(\frac{q_{z_a c, z_c a}}{\sum_{a'} q_{z_{a'} c, z_c a'}} \right) \ln\left(g^{*,R}_{c} \right)_a \tag{26}$$

$$\left\langle \ln g^{*,R}_{a} \right\rangle = \sum_{c} \left(\frac{q_{z_a c, z_c a}}{\sum_{c'} q_{z_a c', z_{c'} a}} \right) \ln\left(g^{*,R}_{a} \right)_c \tag{27}$$

where the angular brackets imply average.

Data Regression: Determination of Interaction Parameters

The adjustable parameters were determined by data regression using the ODRPACK data maximum likelihood regression system [13]. Molecule-molecule binary parameters were first adjusted on experimental binary system data reported in the literature. Best values of molecule-

ion pair and ion-pair molecule interaction parameters were then determined by fixing molecule-molecule parameters at previously estimated values and fitting molecule-ion pair parameters on ternary system data reported in the literature. Similarly, ion pair-ion pair interaction parameters were next determined by fixing molecule-molecule and molecule-ion pair parameters at previously estimated values and fitting ion pair-ion pair parameters on quaternary system data. All interaction parameters were assumed to be temperature dependent and were fitted to one of the following functions of temperature:

$$t = a + \frac{b}{T} \; or \; a + cT \tag{28}$$

Results and Discussion

Values of the t 's obtained from the fitting are presented in Table 1. The parameters for protonated amine bicarbonate or carbamate were obtained from CO_2 pressure versus loading in the appropriate amine, while those for the protonated amine bisulfide were obtained from H_2S pressure versus loading. Parameters between bisulfide and bicarbonate or carbamate ion pairs were obtained from data where both acid gases were present. Parameters between MEA and MDEA salts or molecules were obtained from data for CO_2 and mixed amine solutions. Unfortunately no data exist for H_2S and mixed amines, and as a result the remaining ion pair parameters could not be determined.

Figure 1 shows the ratio of the experimental to the predicted values for the equilibrium H_2S partial pressure versus the H_2S loading (moles of H_2S per mole of amine) for MEA solutions. Figure 2 is a similar plot showing the ratio of the experimental to predicted H_2S loading. Figure 3 is a comparison of model predictions versus experimental results for H_2S vapor pressure versus loading for a typical MEA molality at various temperatures. Figure 4 presents a similar result for CO_2 vapor pressure versus loading for an MEA molality, while Figure 5 shows similar results for

CO_2 over MDEA solutions. Figure 6 shows a typical result for systems where two acid gases are present, comparing predicted versus experimental H_2S vapor pressures over aqueous MDEA solutions. Figure 7 shows a comparison of CO_2 vapor pressure versus loading for several aqueous mixtures of MEA + MDEA. In most cases the agreement is fairly good. Deviations occur primarily in the very low loading region where there is very significant scatter in the experimental data. Also, in a number of instances data at low loading are not available. Finally figures 8 and 9 illustrate how the calculated mole fractions and activity coefficients of all components vary with loading for these solutions.

Results presented above indicate that the electrolyte UNIQUAC model, using ion-pair interactions, is able to adequately represent the phase equilibrium data for the CO_2-H_2S-MEA-MDEA aqueous system. The ion-pair interaction approach results in a model with fewer required interaction parameters than the ion-specific model, yet is algebraically much simpler than the local-electroneutrality assumption used in the electrolyte-NRTL model.

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Table 1. Binary Interaction Parameters of CO_2-H_2S-MEA-MDEA-Water System,

For $\tau_{i,j} = a_{i,j} + b_{i,j}/T$ or $a_{i,j} + c_{i,j} T$, *T* is temperature in degree Kelvin

Binary Components, i,j	$a_{i,j}$	$b_{i,j}$ or $c_{i,j}$	$a_{j,i}$	$b_{j,i}$ or $c_{j,i}$
H_2O-MEA	40.16	-39493.26 /T	-202.45	3594.63 /T
H_2O-MDEA	714.14	-2.93 *T*	-2477.48	7.56 *T*
H_2O-CO_2	-10926.25	-3274442.31/T	-554.08	166018.51/T
H_2O-H_2S	545.80	–176181.73/T	-172.304	88077.51/T
H_2O-$MEAH^+$,HCO_3^-	148.46	.000348 /T	91.06	.001963 /T
MEA-$MEAH^+$,HCO_3^-	.007451	0	.87703	0
MEA-$MEAH^+$,$MEACOO^-$	-21.51	0	.000027	0
H_2O-$MEAH^+$,$MEACOO^-$	2.87	- .000121 / *T*	233.19	- .000123 / *T*
H_2O-$MEAH^+$,HS^-	1600.5	–321300 / *T*	-904.2	170200 / *T*
MEA-$MEAH^+$,HS^-	775.2	–261800 / *T*	-704.7	209400 / *T*
H_2S-$MEAH^+$, HS^-	4458.1	-1378 000 / *T*	26000	1000 / *T*
H_2O-$MDEAH^+$,HCO_3^-	4060.9	-13.61 *T*	152.13	7.99 *T*
MDEA-$MDEAH^+$,HCO_3^-	-2592.34	9.13 *T*	-7.27	1.60 *T*
CO_2-$MDEAH^+$,HCO_3^-	138.49	-1.38 *T*	-4.68	1.34 T
MDEA-CO_2	-1127.43	0.26 *T*	2827.4	4.45 *T*
H_2O-$MDEAH^+$,HS^-	15994.24	-51.86 *T*	1403.76	-5.91 *T*
MDEA-$MDEAH^+$,HS^-	2182.86	-0.0025 *T*	42.32	-0.0006 *T*
H_2S-$MDEAH^+$,HS^-	47.44	-0.009 *T*	87.0	-178.1 *T*
MDEA-H_2S	-1152.76	0.0004 *T*	3310.5	-0.002 *T*
$MEAH^+$,HCO_3^--$MEAH^+$,HS^-	2101.21	99.97 / *T*	0	195.2 / *T*
$MEAH^+$,HS^--$MEAH^+$,$CRBM^-$	0	-221.34 / *T*	0	0
H_2S-$MDEAH^+$,HCO_3^-	75.985	0	-19.738	0
$MDEAH^+$,HCO_3- $MDEAH^+$,HS^-	89.136	0	-15.267	0.5 *T*
MEA-MDEA	351.23	-.3571 *T*	-16241.1	52.55 *T*
MEA-$MDEAH^+$,HCO_3	123.46	-125.0 *T*	114.5	0
MEAH+,HCO_3^--$MDEAH^+$,$MEACOO^-$	-51.23	0	153.45	240.56 *T*
$MDEAH^+$,HCO_3^--$MEAH^+$,HCO_3^-	13671.27	96.65 *T*	51.254	0

Figure Captions:

Figure 1. Comparison of predicted and reported experimental values of H_2S equilibrium partial pressure over aqueous MEA solutions, • - [14],o, ♦- [15], ◊ - [16].

Figure 2. Comparison of predicted and reported experimental H_2S loading over aqueous MEA solutions, • - [14],o, ♦- [15], ◊ - [16].

Figure 3. Comparison of model predictions (solid curves) with experimental data for H_2S equilibrium partial pressure over 2.5 M MEA solution, •, △, o, ▼, €, ◊, - [14], ▲, ■, ◆- [15].

Figure 4. Comparison of model predictions (solid curves) with experimental data for CO_2 equilibrium partial pressure over 5.0 M MEA solution, ■ - [16], •, o- [17], ◆, ▲, △- [18].

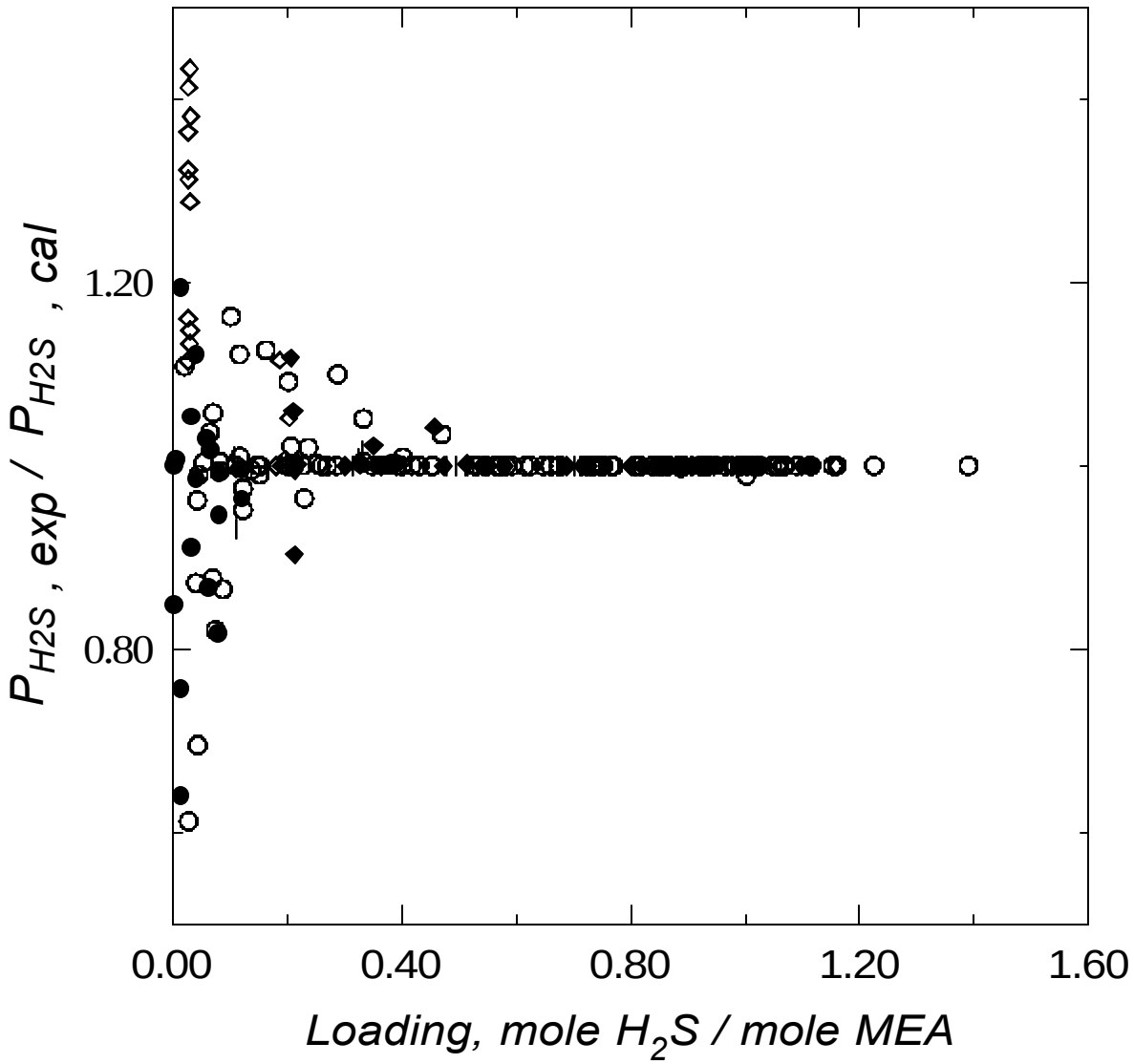
Figure 5. Comparison of model predictions (solid curves) with experimental data for CO_2 equilibrium partial pressure over 23 wt% MDEA solution, ◊ - [6], •, ▲, ■, ◆ - [19], △, o, €, ▽ - [16] .

Figure 6. Comparison of predicted and reported experimental values of H_2S equilibrium partial pressure over aqueous MDEA solutions, o - [20], € - [21].

Figure 7. Comparison of model predictions (curves) with experimental data for CO_2 equilibrium partial pressure over 30 wt % MEA-MDEA aqueous mixtures, • - 12 wt. % MEA, 100 ° C, o - 24 wt. % MEA, 100 ° C, ▲ - 6 wt. %, 60 ° C, △ - 18 wt. % MEA, 40 ° C [22] .

Figure 8. Liquid-phase compositions of a mixed amine solution loaded with CO_2 at 40°C.

Figure 9. Activity coefficients of the various species in a mixed amines solution loaded with CO_2 at 40°C.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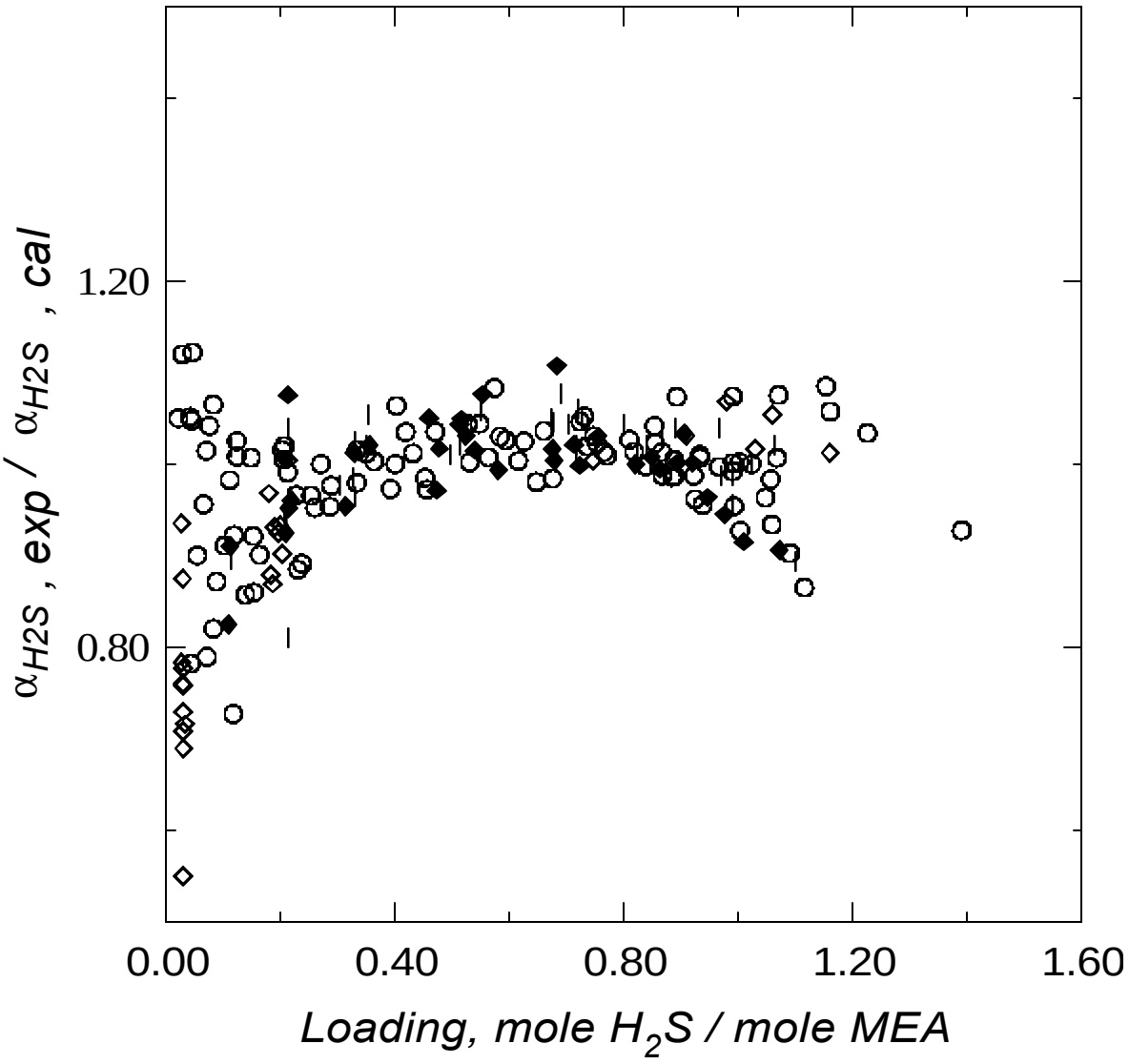
1.20
1.60
Loading, mole H_2S / mole MEA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α_{H2S} , exp / α_{H2S} , cal
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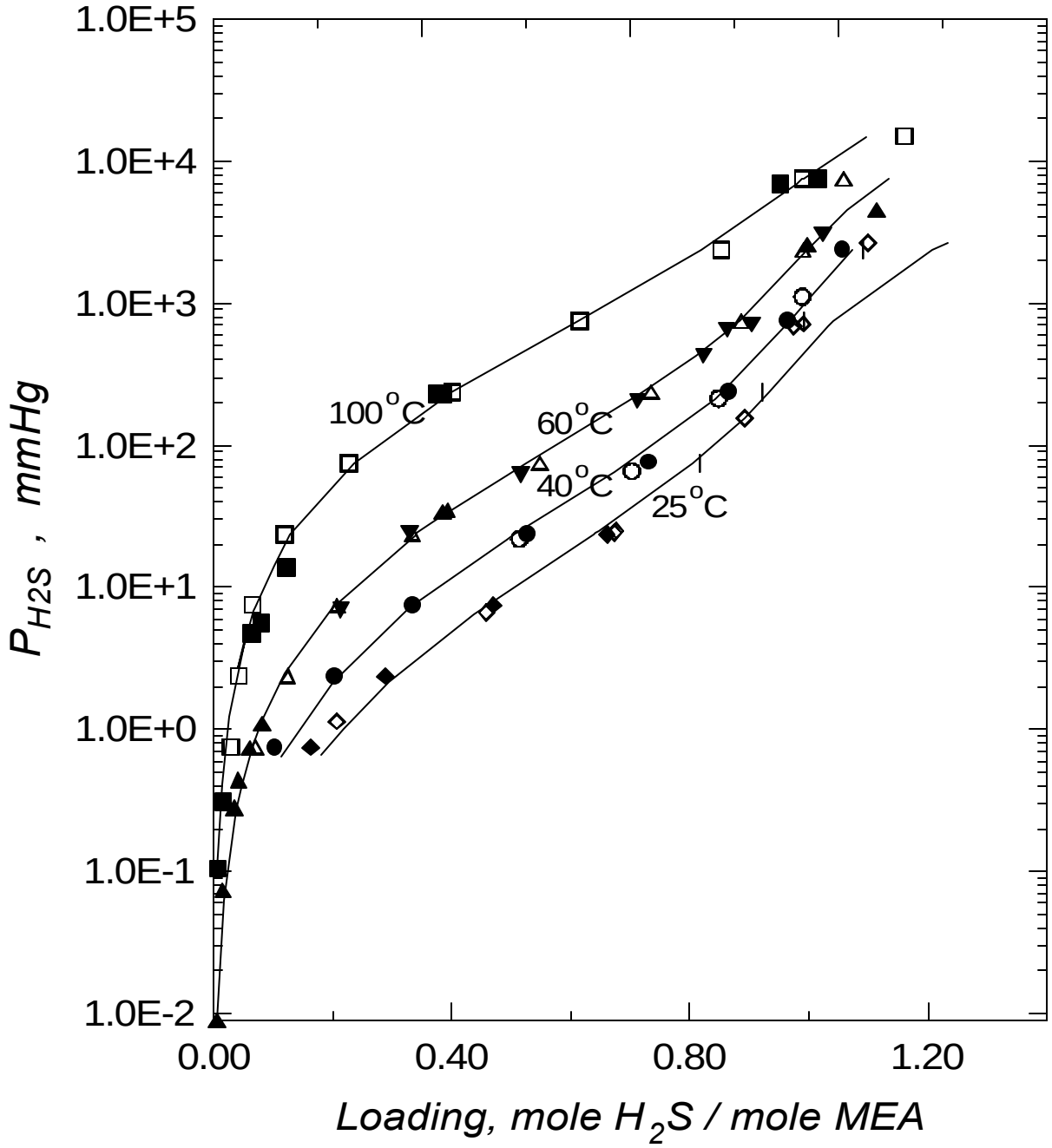
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1.0E+2
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1.0E-1
1.0E-2
P_{H2S} , mmHg
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60°C
40°C
25°C
0.00
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0.80
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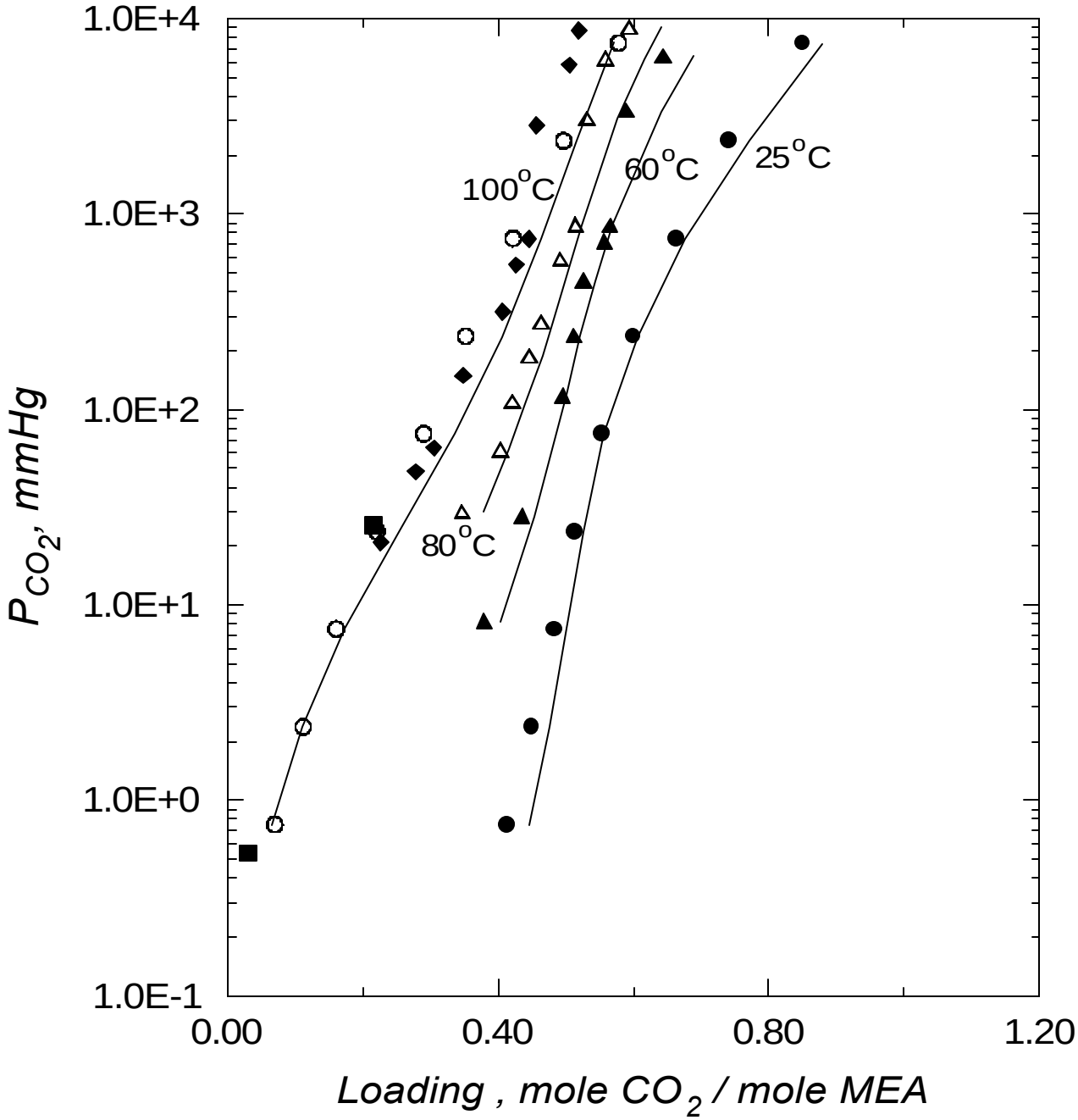
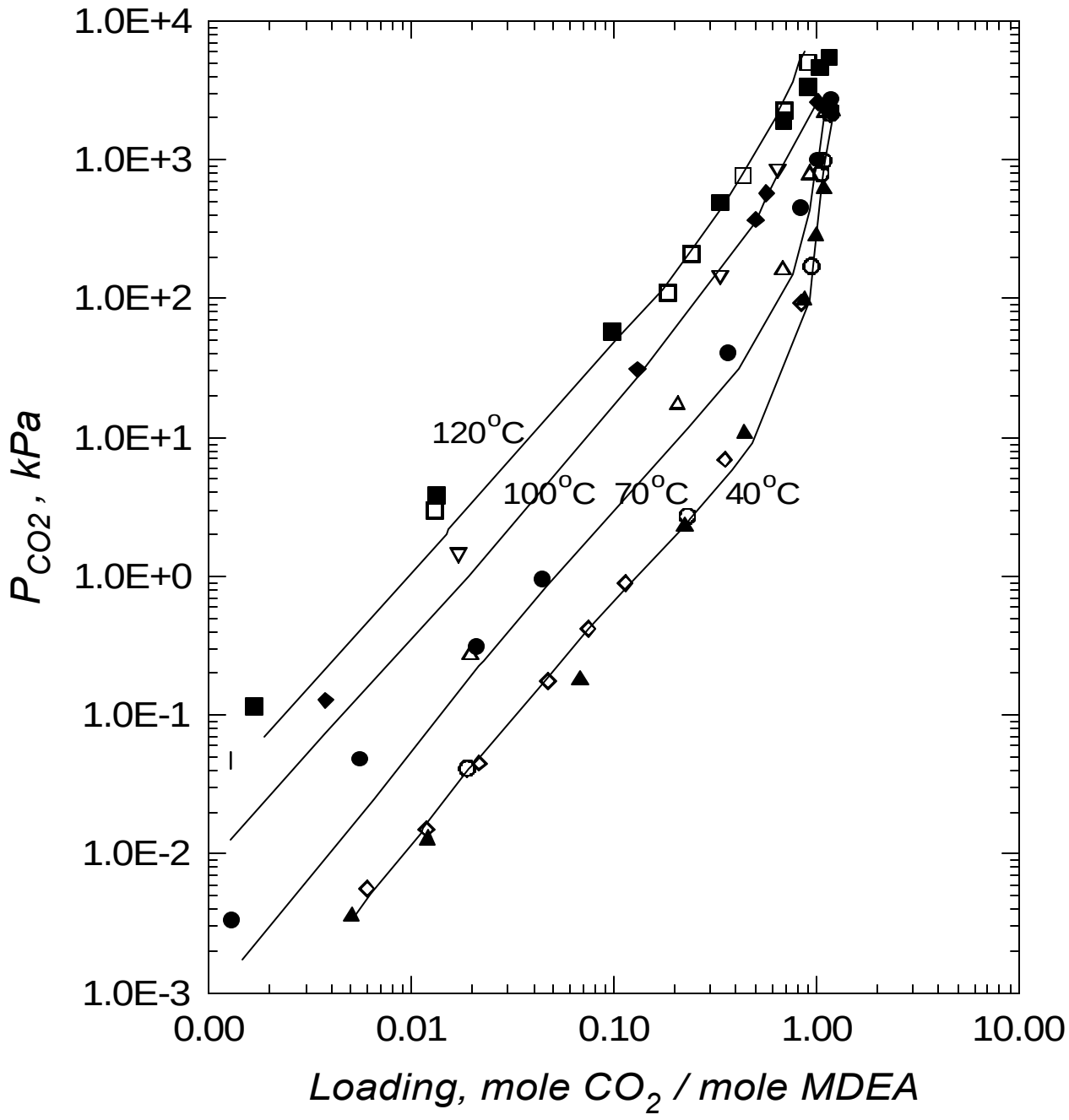
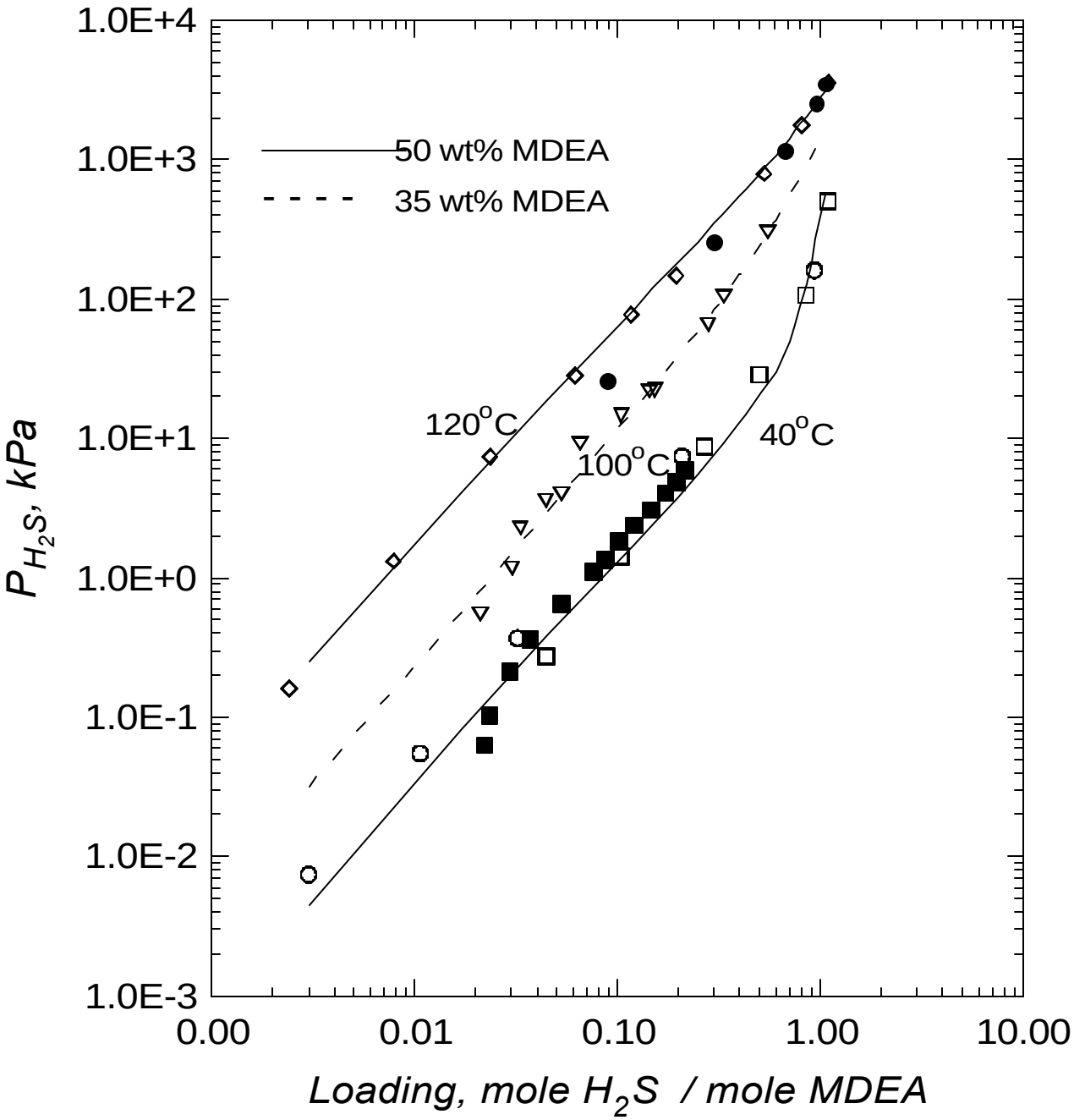
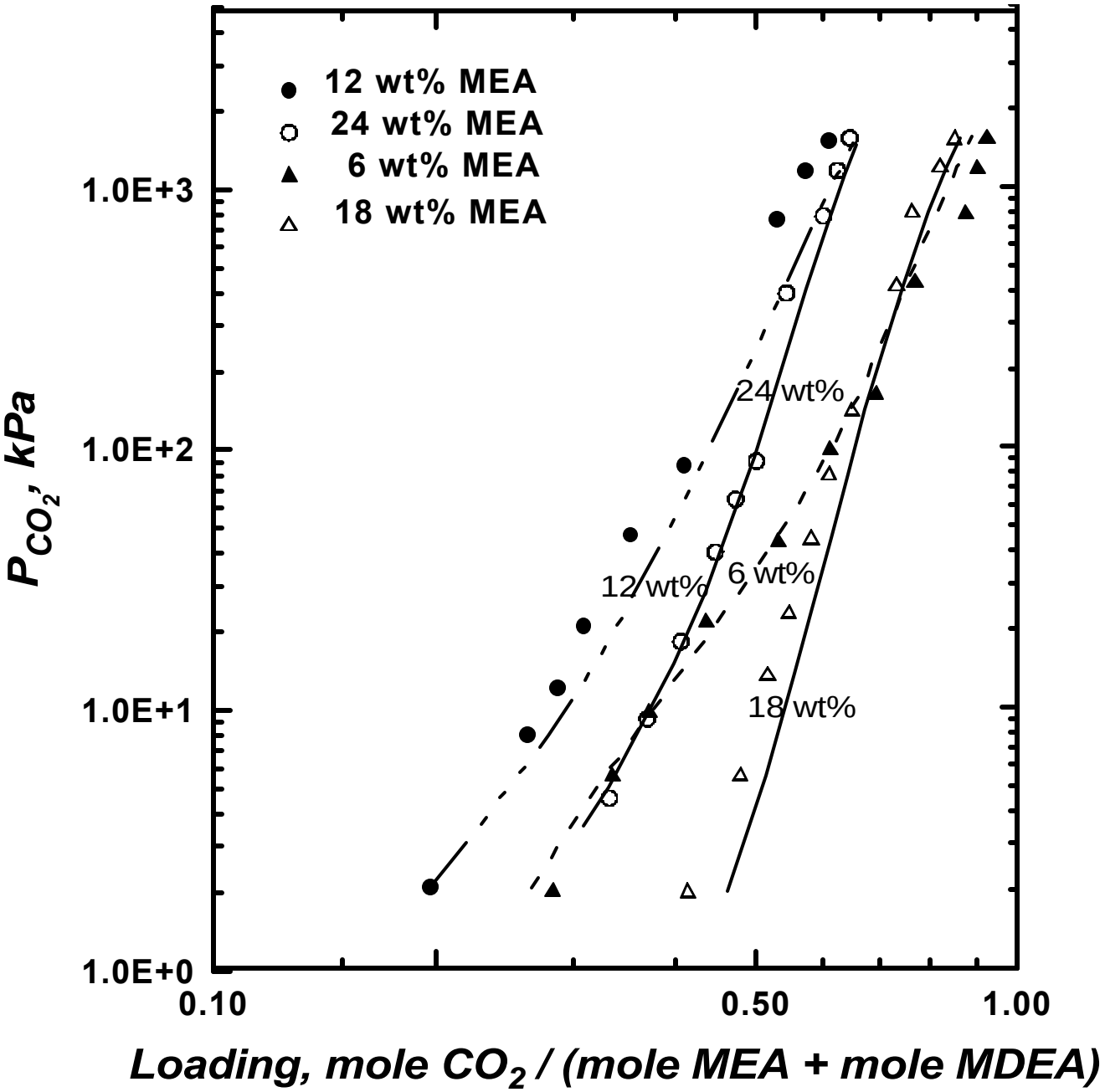
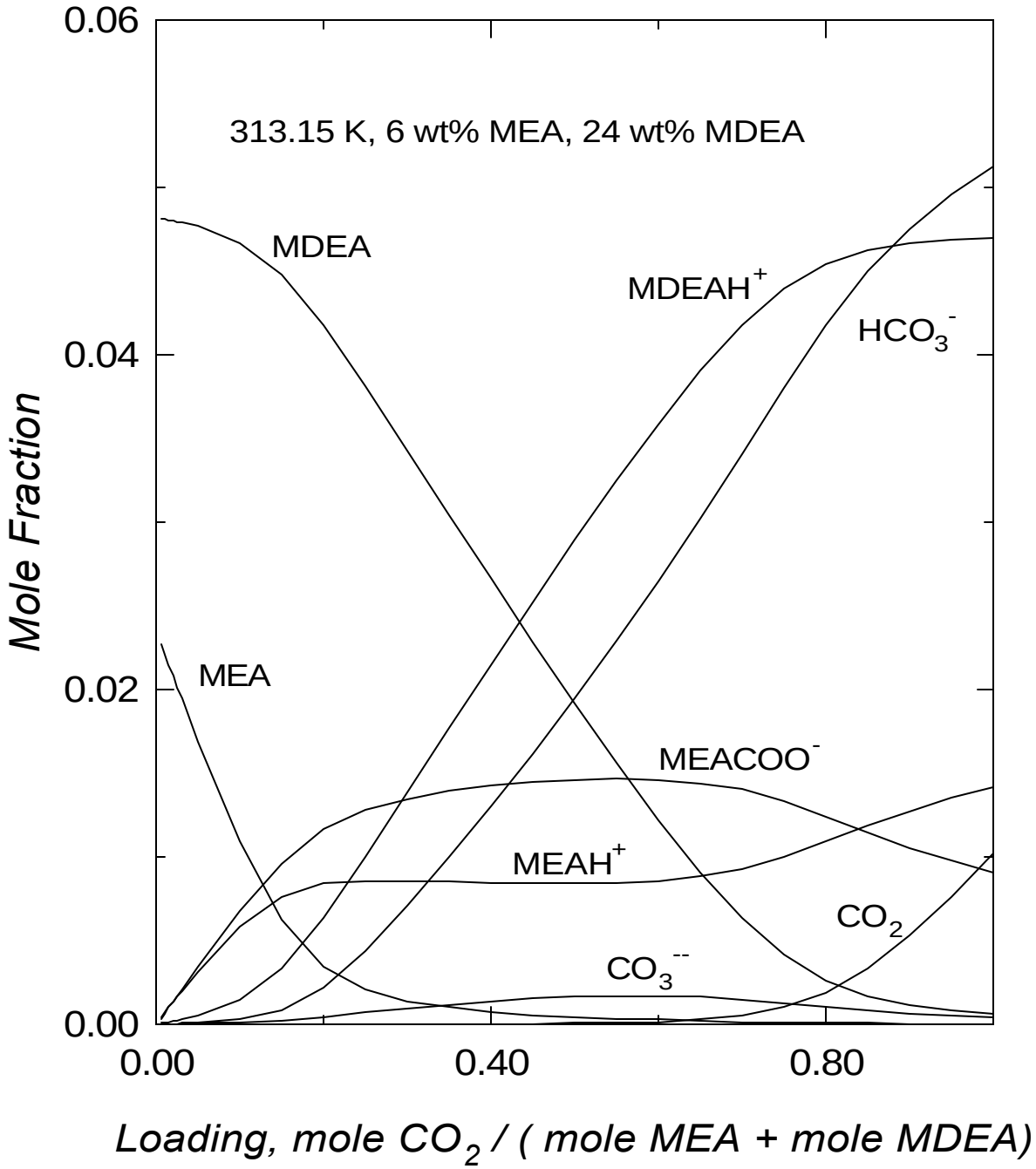
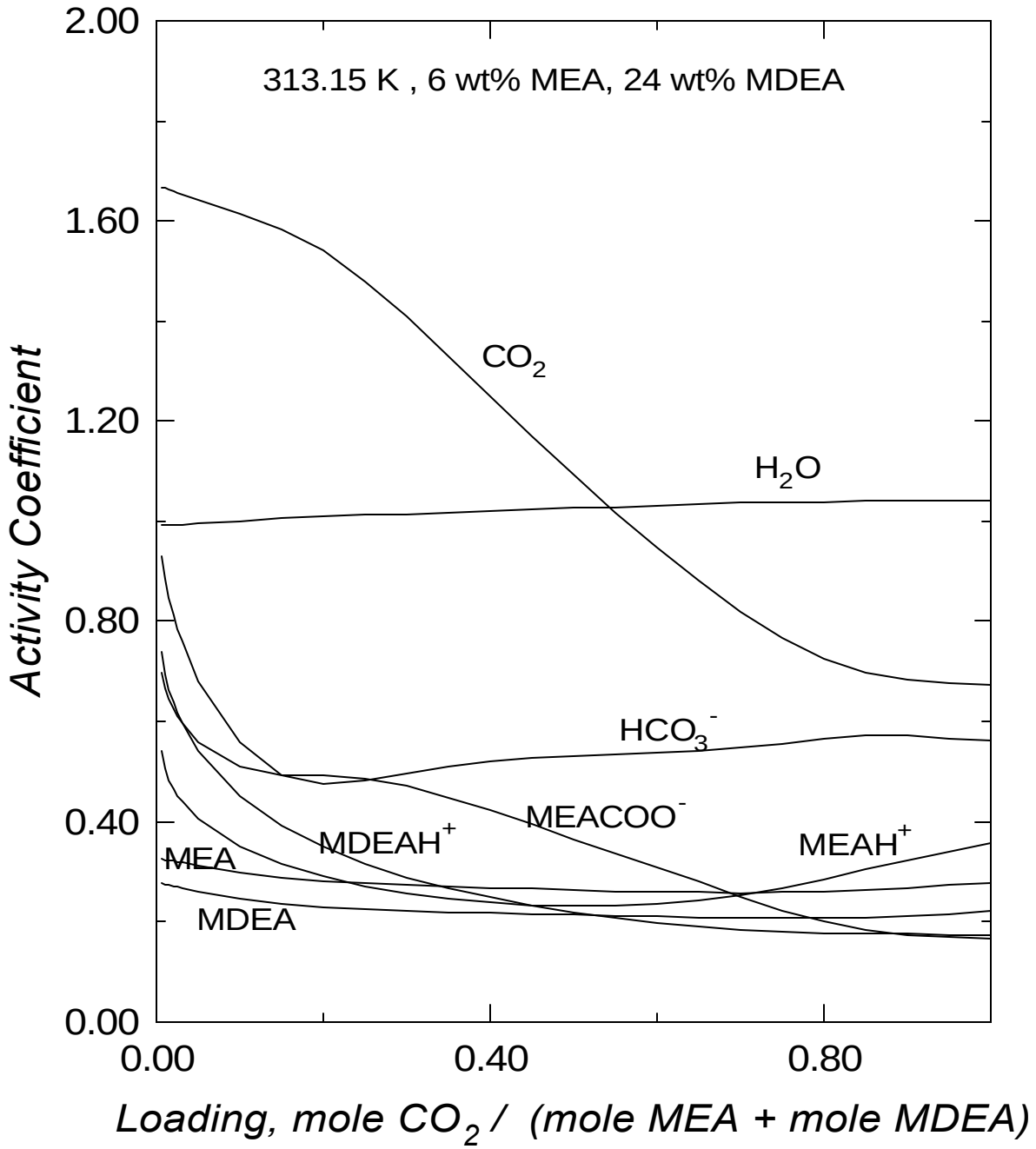

1.0E+4
1.0E+3
1.0E+2
1.0E+1
1.0E+0
1.0E-1
P_{CO_2}, mmHg
0.00
0.40
0.80
1.20
Loading , mole CO_2 / mole MEA
100°C
80°C
60°C
25°C


1.0E+4
1.0E+3
1.0E+2
1.0E+1
1.0E+0
1.0E-1
1.0E-2
1.0E-3
P_{CO2}, kPa
120°C
100°C
70°C
40°C
0.00
0.01
0.10
1.00
10.00
Loading, mole CO_2 / mole MDEA


1.0E+4
1.0E+3
1.0E+2
1.0E+1
1.0E+0
1.0E-1
1.0E-2
1.0E-3
0.00
0.01
0.10
1.00
10.00
50 wt% MDEA
35 wt% MDEA
120°C
100°C
40°C
P_{H_2S}, kPa
Loading, mole H_2S / mole MDEA


12 wt% MEA
24 wt% MEA
6 wt% MEA
18 wt% MEA
1.0E+3
1.0E+2
1.0E+1
1.0E+0
0.10
0.50
1.00
P_{CO_2}, kPa
Loading, mole CO_2 / (mole MEA + mole MDEA)
24 wt%
12 wt%
6 wt%
18 wt%


313.15 K, 6 wt% MEA, 24 wt% MDEA
MDEA
MDEAH+
HCO3-
MEA
MEACOO-
MEAH+
CO2
CO3--
0.06
0.04
0.02
0.00
0.00
0.40
0.80
Mole Fraction
Loading, mole CO2 / (mole MEA + mole MDEA)


313.15 K , 6 wt% MEA, 24 wt% MDEA
2.00
1.60
1.20
0.80
0.40
0.00
0.00
0.40
0.80
Activity Coefficient
Loading, mole CO2 / (mole MEA + mole MDEA)
CO2
H2O
HCO3-
MEACOO-
MDEAH+
MEAH+
MEA
MDEA